

Linear optical susceptibilities of the oxoborate $(\text{Pb}_3\text{O})_2(\text{BO}_3)_2\text{WO}_4$: Theory and experiment

Abstract

The optical susceptibilities have been investigated experimentally and theoretically for a newly synthesized oxoborate, $(\text{Pb}_3\text{O})_2(\text{BO}_3)_2\text{WO}_4$. The crystal structure is composed of one-dimensional $[\text{Pb}_3\text{O}]^{4+}$ chains formed by corner-sharing OPb_4 tetrahedra. BO_3 and WO_4 groups are located around the chains to hold them together via Pb-O bonds. The solid-state fluorescence spectrum exhibited a maximum emission peak at around 375.2 nm with excitation light of 280 nm. UV-Vis diffuse reflectance spectra showed a band gap of about 2.9 eV which compares well with our theoretical band gap of about 2.3 eV obtained using the local density approximation and 2.6 eV using the Engel-Vosko's generalized gradient approximation. We have optimized the atomic positions starting from our X-ray diffraction data so as to minimize the forces on each atom. A remarkable finding is that this crystal possesses a weak anisotropy among three components of the frequency-dependent dielectric function and a small positive birefringence. This indicates that the oxoborate, $(\text{Pb}_3\text{O})_2(\text{BO}_3)_2\text{WO}_4$, cannot be used to produce second harmonic generation (SHG) and optical parametric oscillation.